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ON HIGHER ORDER DYNAMICS IN LATTICE-BASED MODELS USING CHAPMAN-ENSKOG METHOD

YUE-HONG QIAN* AND YE ZHOU†

Abstract. In this paper, we investigate the existence of higher order dynamics in lattice-based models. We have identified two conditions that determine whether a model would allow some Burnett-like equations when the Chapman-Enskog expansion is used. These two conditions are the number of the conserved quantities as well as the space and time discretization. We shall demonstrate these conditions by discussing (1) pure diffusion equation, and (2) hydrodynamic equations. While the fact that diffusion equation allows the higher order dynamics can be shown easily, we will illustrate that care must be taken when deriving Burnett-like equations for lattice-based hydrodynamics models using the Chapman-Enskog method.

Key words. Boltzmann equation, lattice-based hydrodynamics models, Navier-Stokes equation

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1. Introduction. Compared to traditional methods in computational fluid dynamics (CFD), the lattice-based models are simple and easy to implement on computers. The advantages and disadvantages of the original lattice gas automata (LGA) have been well documented [1-7]. The lattice Boltzmann equation (LBE) was later introduced to remove some of the drawbacks [8-10]. A further simplification to the LBE is achieved using the BGK procedure (LBGK) [11-14].

In lattice-based models, it is well established that the Navier-Stokes equation can be deduced at low order expansion of Chapman-Enskog expansion [15]. Many authors further asserted that the Burnett-like equation could be obtained by performing higher order using Chapman-Enskog expansion [4,6,7]. The motivation of this paper is to carry out these higher order Chapman-Enskog expansion to investigate whether it is consistent to do so. We will first study the lattice-based model for pure diffusion model [16,17]; and demonstrate that higher order dynamics is allowed in this case. We will then point out that the Burnett-like equations could be derived for lattice-based hydrodynamics models. Attention should be paid, however, when the classic Chapman-Enskog expansion is applied because of the non-commutative feature of cross derivatives of two time scales, these derivatives do not exist in the continuous time and space while do exist in discrete velocity models [18]. The number of conserved quantities is also critical for the existence of higher order equations.

2. High Order Dynamics: Pure Diffusion. We now consider the lattice BGK models for pure diffusion problems where the only quantity conserved during the redistribution is the total mass. The propagation step is the same as lattice gas models while the collision step is just a redistribution of mass in all possible directions. We start with the following evolution equation [12],

$$f_i(\vec{x}+\vec{c}_i, t+1) = f_i(\vec{x}, t) + \omega(f_i^{eq}(\vec{x}, t) - f_i(\vec{x}, t)) \tag{2.1}$$

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where f_i is the average population of particles with velocity $\vec{c}_i (i = 1, 2, ..., B)$ which belongs to a predetermined finite set and ω the relaxation parameter which satisfies $0 \leq \omega \leq 2$. The local equilibrium population $f_i^{eq}(\vec{x}, t)$ is chosen as [17],

$$f_i^{eq}(\vec{x}, t) = w_i \rho(\vec{x}, t), \qquad w_i = \frac{1}{B}. \tag{2.2}$$

B is the number of particles' discrete velocities. This is a homogeneous equilibrium population in all velocity directions. The macroscopic density, denoted by ρ, is defined by:

$$\rho(\vec{x}, t) = \sum_{i=1}^{B} f_i(\vec{x}, t) = \sum_{i=1}^{B} f_i^{eq}(\vec{x}, t). \tag{2.3}$$

The weighting factor w_i satisfies the normalization constraint: $\sum_i^B w_i = 1$. The choice (2.2) for the equilibrium population, when used together with (2.1) and (2.3), will be shown to lead to the diffusion equation. We consider models with the particle velocity set in D dimension ($D = 1, 2$ and 3). The simplest models take the velocity set of $2D$ elements: D directions along axis and D opposite directions. The rest particles can also be included.

We assume a weak deviation from the local equilibrium $f_i^{eq}(\vec{x}, t)$,

$$f_i(\vec{x}, t) = f_i^{eq}(\vec{x}, t) + \epsilon f_i^{(1)}(\vec{x}, t) + \epsilon^2 f_i^{(2)}(\vec{x}, t) + \cdots \tag{2.4}$$

where ϵ is the appropriate Knudsen number. The space and time derivatives are expressed in terms of multiple-scale variables up to the fourth order in time (see, for example, Huang [19]),

$$\partial_\alpha = \epsilon \partial_\alpha \tag{2.5}$$

$$\partial_t = \epsilon \partial_{t_1} + \epsilon^2 \partial_{t_2} + \epsilon^3 \partial_{t_3} + \epsilon^4 \partial_{t_4}. \tag{2.6}$$

When the total mass is conserved, it follows from (2.1), (2.2), (2.3) and (2.4) that,

$$\sum_{i=1}^{B} f_i^{(j)} = 0, \qquad j > 0. \tag{2.7}$$

Using the classic Chapman-Enskog expansion and taking into account of the discreteness of lattice model, we obtain the first order equation in ϵ,

$$\partial_{t_1} \rho = 0. \tag{2.8}$$

The second order equation is,

$$\partial_{t_2} \rho - \frac{c^2}{2D}(\frac{2}{\omega} - 1)\partial_{\alpha\alpha}\rho = 0. \tag{2.9}$$

The equations (2.8) and (2.9), i.e., the dynamical equations from the two separated time scales $1/\epsilon$ and $1/\epsilon^2$, are now reconstituted to obtain the macro-dynamical equations for the model. The equation of diffusion equation is obtained from (2.8) and (2.9)

$$\partial_t \rho = \kappa_2 \partial_{\alpha\alpha} \rho \tag{2.10}$$

where the diffusivity κ_2 is given by

$$\kappa_2 = \frac{c^2}{2D}(\frac{2}{\omega} - 1). \tag{2.11}$$

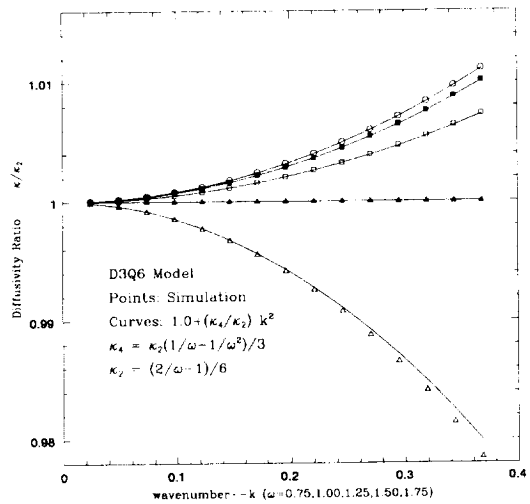

FIG. 2.1. *The dispersion relation (up to fourth order)* $\frac{\kappa}{\kappa_2}$ *versus* k *for the D3Q6 model, The open triangles, solid triangles, open squares, solid squares and open circles are numerical simulations corresponding to* $\omega = 0.75, 1.0, 1.25, 1.5$ *and* 1.75, *respectively. The critical value* ω_{cr} *is* 1.0 *for this model.*

We can also obtain higher order equations by carrying the Chapman-Enskog expansion further. We derive the third order equation,

$$\partial_{t_3}\rho = 0 \tag{2.12}$$

and the fourth order equation,

$$\partial_{t_4}\rho = -A_1\partial_{\alpha\alpha\beta\beta}\rho - A_2\partial_{\alpha\alpha\alpha\alpha}\rho. \tag{2.13}$$

The coefficients A_1, A_2 and κ_2 in (2.10) for models including rest particles are obtained after some algebraic calculations,

$$\kappa_2 = \frac{c^2}{2D}(\frac{2}{\omega} - 1) \tag{2.14}$$

$$A_1 = \frac{c^2}{D}(\frac{2}{\omega^2} - \frac{2}{\omega} + \frac{1}{4})\kappa_2 \tag{2.15}$$

$$A_2 = c^2(-\frac{1}{\omega^2} + \frac{1}{\omega} - \frac{1}{12})\kappa_2. \tag{2.16}$$

The final fourth order equation is the following [17],

$$\partial_t\rho = \kappa_2\partial_{\alpha\alpha}\rho - A_1\partial_{\alpha\alpha\beta\beta}\rho - A_2\partial_{\alpha\alpha\alpha\alpha}\rho. \tag{2.17}$$

We note that Equation 2.17 is anisotropic due to the last term. Applying the Fourier transform $exp(-\Omega t - ikx)$ (k is the wavenumber and Ω the frequency) to the above equation in one-dimensional space, we get the dispersion relation which reads as,

$$\frac{\kappa}{\kappa_2} = 1 + \frac{\kappa_4}{\kappa_2}k^2, \tag{2.18}$$

where $\kappa_4 = A_1 + A_2$ and $\kappa = \frac{\Omega}{k^2}$.

Numerical result is given by the Figure 2.1. The curves correspond to theoretical results κ/κ_2 while the points correspond to numerical simulations of the lattice model presented above. Satisfactory agreements in all cases are achieved. The fourth order corrections may have effects in the regime of large Knudsen number, i.e., large k and small ω. Equation 2.18 is valid only for wavevector along x (or y, z) axis, so is the critical value $\omega_{cr} = 1$ for the D3Q6 numerical model [12] used for Equation 2.1.

3. High Order Dynamics: Hydrodynamics. We now turn our attention to lattice-based hydrodynamics models. In the LGA, LBE, and LBGK models, both the mass and momentum are conserved. The common features in these models are discrete velocity space of particles, evolution steps of local interactions and neighbor-to-neighbor propagation of moving particles. Since the principle of deriving large-scale equations is the same and outlined in the previous section. For the sake of simplicity, we use lattice BGK models to illustrate the existence of high order dynamics: Burnett-like equations. In classic kinetic theory, Euler, Navier-Stokes, Burnett and Super-Burnett equations constitute the successive approximations of the Boltzmann equation in the order of Knudsen number. Like in classic kinetic theory, the lattice-based models for hydrodynamics use the Chapman-Enskog expansion in order to derive the Navier-Stokes equations. We outline the basic ingredients of the derivation. The time evolution equation is the same as section 2, except that the equilibrium distribution f_i^{eq} contains not only mass, but also momentum,

$$f_i^{eq} = t_p\rho(1 + \frac{c_{i\alpha}u_\alpha}{c_s^2} + \frac{(c_{i\alpha}c_{i\beta} - c_s^2\delta_{\alpha\beta})u_\alpha u_\beta}{2c_s^4}) \tag{3.1}$$

where c_s is a constant. The density ρ and velocity $\vec{u}$ are defined by,

$$\sum_{i=1}^{B} f_i = \sum_{i=1}^{B} f_i^{eq} = \rho, \qquad \sum_{i=1}^{B} \vec{c_i} f_i = \sum_{i=1}^{B} \vec{c_i} f_i^{eq} = \rho\vec{u} \tag{3.2}$$

which leads to the constraints on high order corrections $f_i^{(j)}$,

$$\sum_{i=1}^{B} f_i^{(j)} = 0, \qquad \sum_{i=1}^{B} \vec{c_i} f_i^{(j)} = 0, \qquad j > 0. \tag{3.3}$$

The leading order on ϵ yields the inviscid fluid equations,

$$\partial_{t_1}\rho + \partial_\alpha(\rho u_\alpha) = 0 \tag{3.4}$$

$$\partial_{t_1}(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = -c_s^2\partial_\alpha\rho \tag{3.5}$$

and the second order ϵ^2 results in the dissipative terms,

$$\partial_{t_2}\rho = 0 \tag{3.6}$$

$$\partial_{t_2}(\rho u_\alpha) = \nu(\partial_{\beta\beta}(\rho u_\alpha) + \partial_{\alpha\beta}(\rho u_\beta)) \tag{3.7}$$

where ν is the shear viscosity ($\nu = c_s^2(1/\omega - 1/2)$).

Now, in order to obtain high order hydrodynamical equations of the lattice-based models, let us look at the third order ϵ^3, the Taylor expansion gives the following equation,

$$\partial_{t_3} f_i^{eq} + c_{i\alpha}\partial_\alpha f_i^{(2)} + \partial_{t_1} f_i^{(2)} + \partial_{t_2} f_i^{(1)} + \frac{1}{2}(\underline{\partial_{t_1 t_2} + \partial_{t_2 t_1}} + 2c_{i\alpha}\partial_{t_2\alpha}) f_i^{eq} +$$

$$\frac{1}{2}(\partial_{t_1 t_1} + 2c_{i\alpha}\partial_{t_1\alpha} + c_{i\alpha}c_{i\beta}\partial_{\alpha\beta}) f_i^{(1)} + \frac{1}{6}(\partial_{t_1 t_1 t_1} + 3c_{i\alpha}\partial_{t_1 t_1\alpha} + 3c_{i\alpha}c_{i\beta}\partial_{t_1\alpha\beta} + c_{i\alpha}c_{i\beta}c_{i\gamma}\partial_{\alpha\beta\gamma}) f_i^{eq}$$

$$= -\omega f_i^{(3)}. \tag{3.8}$$

Summing the underlined cross derivative $\partial_{t_1 t_2} f_i^{eq}$ in the above equation over i, we get a term,

$$\partial_{t_1 t_2}(\rho).$$

Using the first and second order Equations 3.4–3.7, we obtain two different results,

(1). if we first take the derivative over t_2 then t_1, we have,

$$\partial_{t_2 t_1}(\rho) = 0.$$

(2). Reversely, we have,

$$\partial_{t_1 t_2}(\rho) = -\nu\partial_\alpha(\partial_{\beta\beta}(\rho u_\alpha) + \partial_{\alpha\beta}(\rho u_\beta))$$

It means that the operators are not commutative,

$$\partial_{t_1 t_2}(\bullet) \neq \partial_{t_2 t_1}(\bullet)$$

where $\bullet$ is either ρ or ρu_α.

Note that[1] the third order macroscopic equations can be also obtained by the wavevector expansion (see for example, van Coervorden *et al.* [20]). Even though the above-mentioned operators are not commutative, the essential point in the Equation 3.8 is the sum of the two terms. After a tedious algebraic calculation, we get the third order equations,

$$\partial_{t_3}\rho = \frac{c_s^2}{6}\partial_{\alpha\beta\beta}(\rho u_\alpha) \tag{3.9}$$

$$\partial_{t_3}(\rho u_\alpha) = \frac{c_s^4}{6}(\frac{12}{\omega^2} - \frac{12}{\omega} + 1)\partial_{\alpha\beta\beta}(\rho). \tag{3.10}$$

We check the dispersion relation up to the third order numerically in Figure 3.1 (the curves are theoretical predictions with Equations 3.9–3.10 and points numerical simulations). Good agreement is obtained.

Even higher order (fourth and up) dynamics can be obtained while tremendous care has to be taken since more non-commutative operators are involved and results will be published elsewhere.

4. Concluding Remarks. In this paper, we pointed out that two conditions determine whether the lattice-based models could or could not have higher order dynamics when classical Chapman-Enskog expansion is used. These conditions are number of conservation laws and the space and time discretization. The pure diffusion model, a system with only one conserved quantity, is first presented to illustrate that the higher order dynamics is allowed. We then turned our attention to the lattice-based hydrodynamics equations. With more than one conserved quantities, we note that special care must be taken to derive governing equations for higher order dynamics. After noting the feature of no-commutative cross time derivative, we demonstrate how Burnett-like equations could be obtained for lattice-based hydrodynamics models using the classic Chapman-Enskog expansion method. The results reported in this paper can be used to analyze theoretically systems where hydrodynamic description may break down, a typical example is simulations of the micro-electronic mechanical systems (MEMS) [21,22].

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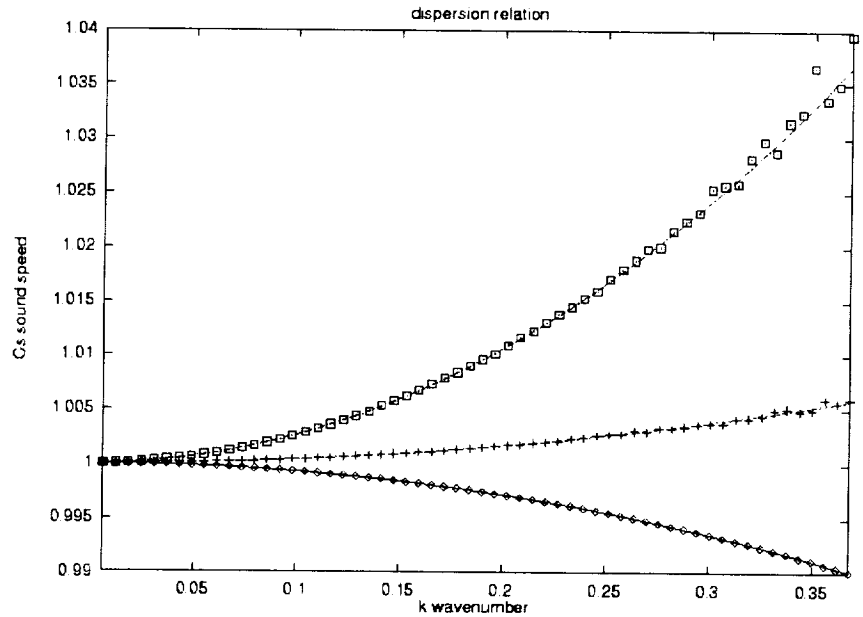

FIG. 3.1. *The dispersion relation (up to third order): The speed of sound versus k for the D1Q5 model, The open triangles, solid triangles, open squares, solid squares and open circles are numerical simulations corresponding to $\omega = 0.75, 1.00$, and* 1.50 *while the curves are theoretical predictions.*

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